JOURNAL OF APPLIED PHYSICS VOLUME 38, NUMBER 6 MAY 1967

The Voigt–Reuss–Hill Approximation and Elastic Moduli of Polycrystalline MgO, CaF_2, β-ZnS, ZnSe, and CdTe

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(Received 15 December 1966; in final form 23 January 1967)

The Voigt–Reuss–Hill (VRH) approximation, a useful scheme by which anisotropic single-crystal elastic constants can be converted into isotropic polycrystalline elastic moduli, is shown to apply for moderately anisotropic cubic crystals like MgO, CaF_2, β-ZnS, ZnSe, and CdTe. Experimental values of polycrystalline isotropic elastic moduli for these materials are presented here, and the validity of the VRH approximation is established. The VRH approximation is then discussed for these materials with respect to their elastic anisotropy of crystals. To provide further support to this work, a numerical confirmation on the VRH moduli is made with the use of a high-speed computer by calculating the mean velocity of sound in crystals and comparing this result with the corresponding quantity calculated from the actual polycrystalline elastic moduli. The general agreement is observed.

1. INTRODUCTION

The Voigt–Reuss–Hill approximation is an averaging scheme by which anisotropic single-crystal elastic constants can be converted into isotropic polycrystalline elastic moduli. The averaging scheme is explicitly based on three independent theoretical contributions due to Voigt,[1] Reuss,[2] and Hill[3]; thus it was named the Voigt–Reuss–Hill (VRH) approximation.[4,5] The VRH approximation is simple and easily tractable in theory. For a single-phase crystalline aggregate made of crystals that are slightly anisotropic, the approximation gives the realistic values of isotropic elastic moduli. However, for aggregates containing crystals of highly anisotropic crystals, a question arises whether or not this approximation gives still the realistic estimates of the polycrystalline elastic properties.

The purpose of this paper is to study the VRH approximation for highly anisotropic cubic crystals and to examine to what extent this approximation is useful for calculating the polycrystalline isotropic moduli from the corresponding single-crystal data. The materials chosen for the present work are MgO, CaF_2, β-ZnS, ZnSe, and CdTe for which the well-characterized polycrystalline specimens were available. The polycrystalline β-ZnS, ZnSe, and CdTe are of particular interest in the present work since they are aggregate examples of highly anisotropic crystals having the same structure, and thus the measurements of the isotropic elastic moduli on these materials provide important empirical data that test the validity of the VRH approximation for high elastic anisotropy.

[1] W. Voigt, *Lehrbuch der Kristallphysik* (B. B. Teubner, Leipzig, 1928), p. 739.
[2] A. Reuss, Z. Angew. Math. Mech. 9, 49 (1929).
[3] R. Hill, Proc. Phys. Soc. (London) 65, 349 (1952).
[4] D. H. Chung, Phil. Mag. 8, [89] 833 (1963).
[5] O. L. Anderson, J. Phys. Chem. Solids 24, 909 (1963). The VRHG (Voigt–Reuss–Hill–Gilvarry) approximation so called by Anderson is exactly the same as the VRH (Voigt–Reuss–Hill) approximation. See, for example, *Physical Acoustics*, edited by W. P. Mason, (Academic Press, New York, 1965), Vol. III-B, Chap. 2.

2. EXPERIMENTAL PROCEDURE

2.1. Specimens

The specimens used in the present work are vacuum hot-pressed polycrystalline aggregates and they are virtually free from porosity. These materials are known under a trade name Irtran, available from the Eastman Kodak Company. The specimens were about 0.635 by 0.953 by 7.620 cm in dimension, sufficiently large enough to make accurate resonance measurements as well as measurements of sound velocities. The faces of each specimen were polished to give a rectangular prism whose sides and ends are square and parallel to ±0.001 cm. Using ultrasonic velocity measurements, each specimen was checked for the elastic isotropy by rotating the transducer crystals on the specimen surface. All the specimens were found to be isotropic for both the longitudinal and shear waves. In the following, a brief description of these specimens is made under each material headings.

A. Polycrystalline MgO

One specimen designated hereafter as IR–MgO is a typical Irtran No. 5 material. The measured density was 3.5819 (±0.0009) g/cm³ at 298°K and it should be compared with the x-ray density of 3.581 in the same unit. The chemical purity of IR–MgO was 99.98% MgO. Minor constituents contained in the specimen were as follows: Si 80, Ca 30, Al 25, Fe 25, Cu 10, Sn 5, Ba less than 3, B less than 10, Ni 5, Na 3, Li 2, Cr 4, K and Sr each less than 1 ppm. The specimen was highly translucent in the visible region, and it had an optical reflectance better than 60% in the 14 to 26 μ range. The measured reststrahlen lattice wavelength was 25.3 (±0.2) μ.[6]

B. Polycrystalline CaF_2

One specimen designated under IR–CaF_2 is a typical of Irtran No. 3 material. The measured density for the

[6] *Kodak Irtran 5 Material*. (Eastman Kodak Company, Rochester, New York, 1963).